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December 5, 2003

201-14880

Mr. Michael O. Leavitt  
Administrator  
U.S. Environmental Protection Agency  
P. O. Box 1473  
Merrifield, VA 22116

RE: Ethylbenzene Panel Test Plan for Polyethylbenzene Bottoms (CAS Number 68987-42-8)

Dear Mr. Leavitt:

The Ethylbenzene Panel of the American Chemistry Council submits this test plan for Polyethylbenzene Bottoms (CAS Number 68987-42-8) under the High Production Volume (HPV) Challenge Program.

In preparing this test plan, the Panel has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. The Panel has conducted a thorough review of the published literature and searched internally for all existing data relevant to this CAS number. In analyzing the adequacy of existing data, the Panel has conducted a thoughtful, qualitative analysis rather than a rote checklist approach. In doing this, the Panel believes it has complied with the principles contained in the October 14, 1999 letter.

If you have any questions, please contact Elizabeth Moran, Manager of the Ethylbenzene Panel at 301 924 2006 or [Elizabeth\\_Moran@americanchemistry.com](mailto:Elizabeth_Moran@americanchemistry.com).

Sincerely yours,

cc: R. Hefter, EPA  
S. Russell, ACC  
J. Keith, ACC

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201-14880A

**HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

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**TEST PLAN**

**For**

**Polyethylbenzene Bottoms**

CAS Number 68987-42-8

**Prepared by:**

**American Chemistry Council  
Ethylbenzene Panel**

**December 4, 2003**

## **EXECUTIVE SUMMARY**

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies who produce Polyethylbenzene Bottoms (CAS number 68987-42-8) have committed to developing screening level human health, environmental effects and fate, and physicochemical data for Polyethylbenzene Bottoms under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program). The Polyethylbenzene Bottoms stream is a co-product of ethylbenzene manufacture and a Class II complex mixture. Since no published data were found and limited unpublished studies were found for HPV endpoints, the screening level studies as listed in Section IV will be conducted. Since this material is unique to the ethylbenzene manufacturing process and does not have a composition common with other HPV materials, it is not feasible to combine this material into a category combining multiple CAS numbers for hazard assessment or HPV testing.

**Ethylbenzene Panel**

**Producers of Polyethylbenzene Bottoms**

ATOFINA Petrochemicals Inc.

BP Amoco Chemical Company

Chevron Phillips Chemical Company LP

The Dow Chemical Company

Lyondell Chemical Company

NOVA Chemicals Inc.

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# **TEST PLAN FOR POLYETHYLBENZENE BOTTOMS**

## **I. INTRODUCTION**

The Ethylbenzene Panel (Panel) of the American Chemistry Council and the Panel's member companies who produce Polyethylbenzene Bottoms (PEB HPV Task Group) have committed to develop screening level human health, environmental effects and fate, and physicochemical data for Polyethylbenzene Bottoms under the Environmental Protection Agency's (EPA's) High Production (HPV) Challenge Program (Program).

In preparing this test plan, the PEB HPV Task Group has given careful consideration to the principles contained in the letter EPA sent to all HPV Challenge Program participants on October 14, 1999. As directed by EPA in that letter, the Panel has conducted a thorough search for existing data and a thoughtful, qualitative analysis of the adequacy of existing data. The Panel has taken the same thoughtful approach when developing its test plan. The Panel believes its test plan conforms to the principles articulated in EPA's letter.

The Panel conducted a search of the published literature and found no test data on this material. Panel members searched company files for unpublished data and found data on endpoints that are not part of the HPV dataset (e.g. irritation) or the data were not sufficiently robust to meet the standards of the HPV program. The Panel also considered whether this material could be combined in a category with other HPV chemicals for purposes of the HPV program, but since this material is unique to the ethylbenzene manufacturing process and does not have a composition common with other HPV materials, it is not feasible to combine this material into a category combining multiple CAS numbers for hazard assessment or HPV testing.

Polyethylbenzene Bottoms is identified by CAS number 68987-42-8. No adequate existing data were found in the published literature. Limited data applicable to the HPV endpoints were obtained in the form of unpublished reports sponsored by the producers. The objective of the Panel's participation in the HPV program is to identify and develop sufficient test data and/or other information to adequately characterize the human and environmental fate for the category in accordance with the EPA HPV Program. The Panel plans to conduct tests to develop the screening level data.

## **II. DESCRIPTION OF POLYETHYLBENZENE BOTTOMS**

The Polyethylbenzene Bottoms stream is a co-product of ethylbenzene manufacture. Ethylbenzene is produced through alkylation of benzene with ethylene. In addition to the production of ethylbenzene, there are side reactions that involve the reaction of ethylene with ethylbenzene to produce diethylbenzene and further alkylations to produce triethylbenzene and polyethylbenzene. In addition, butylbenzene and other alkylaromatics may be formed in varying

amounts. After the ethylbenzene is removed, the remaining stream is separated into a diethylbenzene-rich stream and a bottoms stream. This co-product bottoms stream is described as Benzene, ethylenated, residues (CAS# 68987-42-8), also called Polyethylbenzene Bottoms or Polyethylbenzene Residue. This material is a Class II complex mixture.

<b>Chemical Name</b>	<b>Other Names</b>	<b>CAS #</b>
Benzene, ethylenated, residues	Polyethylbenzene Bottoms Polyethylbenzene Residue PEB Bottoms PEB Residue	68987-42-8

The composition of Polyethylbenzene Bottoms listed below is based on capillary GC analysis of samples submitted by the eight participating companies to BP Amoco Analytical Technology (BP Amoco, 2000).

<b>Composition</b>	<b>Wt%</b>
Diphenylethanes	15 – 32
Diphenylmethanes	<0.5 – 31
Other diphenylalkanes	7 – 17
Ethyl diphenylethanes & diethylbiphenyls	9 – 21
Polyethylbenzenes	<0.1 – 19
Triethylbenzenes	<1 – 26
Diethylbenzenes (m-, o-, p-)	<0.1 – 4
Butylbenzenes	<0.1
Other alkylbenzenes	9 – 24
PNAs (3-ring)	0.4 – 11
Ethylbenzene	<0.1
Benzene	<0.1
Paraffins/Naphthenes	<0.3
Total of unidentified components each present at <0.1%	3 – 5

Please note that the Diethylbenzene Rich-Streams (CAS Registry #25340-17-4 and 68608-82-2) are currently being tested separately in 2003 under the HPV Chemical Program.

### **III. SUMMARY OF EXISTING INFORMATION**

No published data on Polyethylbenzene Bottoms for HPV endpoints were found following a search of the literature. Although some unpublished reports on some acute studies were reviewed, none of these data were considered adequate for the HPV endpoints. Nonetheless, robust summaries are provided. Polyethylbenzene Bottoms is characterized by low acute oral and dermal toxicity. The acute oral LD<sub>50</sub> for rats was greater than 5.0 g/kg (Gulf Life Sciences

Center, 1985a). Dermal application at 1.0 or 2.0 g/kg on five consecutive days to rats resulted in no mortality (Gulf Life Sciences Center, 1985b); body weights were decreased at both dose levels.

#### IV. TEST PLAN

A sample representing industry production will be tested. Equal quantities of a Polyethylbenzene Bottoms samples obtained from each current producer company will be blended to produce the Polyethylbenzene Bottoms test stream. The composition of the stream will be characterized and the following studies conducted:

<b>Test</b>	<b>Method</b>
<b>Melting Point/Melting Point Range</b>	<b>OECD 102</b>
<b>Boiling Point</b>	<b>OECD 103</b>
<b>Vapor Pressure</b>	<b>OECD 104</b>
<b>Water Solubility</b>	<b>OECD 105</b>
<b>Partition Coefficient (n-octanol/water, shake flask method)</b>	<b>OECD 107</b>
<b>Photodegradation</b>	<b>(Technical Discussion)</b>
<b>Fugacity Model I or III</b>	<b>(Model)</b>
<b>Ready Biodegradability: Manometric Respirometry Test</b>	<b>OECD 301 F</b>
<b>Fish Acute Toxicity Test</b>	<b>OECD 203</b>
<b><i>Daphnia</i> sp., Acute Immobilization Test and Reproduction Test</b>	<b>OECD 202</b>
<b>Algae, Acute Growth Inhibition Test</b>	<b>OECD 201</b>
<b>Bacterial Reverse Mutation Test</b>	<b>OECD 471</b>
<b><i>In vitro</i> Mammalian Chromosome Aberration Test</b>	<b>OECD 473</b>
<b>Combined Repeated Dose Toxicity Study with Reproductive/Developmental Toxicity Screening Test</b>	<b>OECD 422</b>
<b>Hydrolysis</b>	<b>(Technical Discussion)</b>

The chemical composition of the Polyethylbenzene Bottoms streams indicates this stream is not subject to hydrolysis at measurable rates. Therefore, information for this endpoint will be summarized in a technical review document.



## V. REFERENCES

BP Amoco Company, 2000. Unpublished Report for the American Chemistry Council Ethylbenzene Panel (CMA Reference No. EB-60-RES-HPV-BP Amoco). June 7, 2000). BP Amoco Technology Center, Naperville, IL.

Gulf Life Sciences Center. 1985a. Acute oral toxicity study in rats of Polyethylbenzene Bottoms. Project No. 84-2133. Sponsored by Gulf Oil Products Company. Gulf Life Sciences Center, Pittsburgh, PA.

Gulf Life Sciences Center. 1985b. Five-day repeated dose dermal toxicity in rats of Polyethylbenzene Bottoms. Project No. 84-2137. Sponsored by Gulf Oil Products Company. Gulf Life Sciences Center, Pittsburgh, PA.

**Table 1. Assessment Plan for Polyethylbenzene Bottoms.** (Robust summaries provided separately)

	Human Health Effects						Ecotoxicity				Environmental Fate			
Stream Description	Acute Toxicity	Genetic Point Mut.	Genetic Chrom.	Sub-chronic	Developmental	Reproduction	Acute Fish	Acute Invert.	Algal Toxicity	Physical Chem.	Photodeg.	Hydrolysis	Fugacity	Biodeg.
Polyethylbenzene Bottoms	E	T	T	T	T	T	T	T	T	T	TD	TD	M	T

E Existing Data  
T Testing proposed

TD Technical Discussion  
M Model

201-14880B

**HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

**ROBUST SUMMARIES**

**For the**

**Polyethylbenzene Bottoms**

**CAS Number 68987-43-9**

**Prepared by:**

**American Chemistry Council  
Ethylbenzene Panel HPV Task Group  
Polyethylbenzene Bottoms Subteam**

**December 4, 2003**

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## ACUTE ORAL TOXICITY

### Test Substance

Identity: Polyethylbenzene Bottoms (CAS No. 68987-43-9)  
Purity: Not stated

### Method

Method/guideline followed: FIFRA/ TSCA guidelines  
Type: LD<sub>50</sub>  
GLP: Not stated  
Year: 1985  
Species/Strain: Fisher 344 Rat  
Sex: Male and female  
No. of animals per sex per dose: 5  
Vehicle: None  
Route of administration: Oral/ gastric intubation  
Remarks: At the start of experiment, animals were 65 days old with a weight ranging from 113 to 166 grams. During the study, room temperature averaged 72.8°F, and relative humidity averaged 55%. Each animal was observed at 1 hr and 4 hr after administration of the test substance and at least once daily for 14 days post dosing.

### Results

Remarks: >5.0 g/kg  
No mortality was observed during the study. Soft feces were observed at the 4-hour observation and on Days 2 and 3. Anogenital soiling was noted at the 4-hour observation and on Days 2,3, 6 and 8. Brown material around the nose and mouth was seen on some animals on Days 2 and 3. All animals were normal for all clinical observation intervals from Day 9 until study termination.  
  
No adverse effects on body weights were observed throughout the study. Gross necropsies of the animals were performed and the observed tissues were within normal limits for the species.

### Conclusions

Based on the lack of mortality at 5.0 g/kg, PEB was assigned a descriptive classification for acute oral exposure of “practically non-toxic”.

**Data Quality**

Reliability (Klimisch):

1b

Remarks:

Reliable without restrictions, comparable to current guideline study.

**Reference**

Gulf Life Science Center. 1985. Acute Oral Toxicity Study in Rats of Polyethylene Bottoms. Project No. 84-2133

**Other**

Last changed:

October 20, 2003

Remarks:

None

## ACUTE DERMAL TOXICITY

### Test Substance

Identity:	Polyethylbenzene (PEB) Bottoms (CAS No. 6897-43-9)
Purity:	Not stated

### Method

Method/guideline followed:	Other
Type:	Five-day repeated dose
GLP:	Not stated
Year:	1985
Species/Strain:	Fischer 344 Rat
Sex:	Male and female
No. of animals per sex per dose:	5
Vehicle:	Light paraffin oil [CAS # 8012-95-1]
Route of administration:	Dermal
Remarks:	At the start of the experiment, animals were 70 days of age and weighed between 129.27 g to 206.32 g. During the study, animal rooms were maintained at an average ambient temperature of 73.6°F and relative humidity of 55.5%.

Prior to treatment initiation, the backs of all animals were clipped free of hair. Each animal was fitted with an Elizabethan collar to prevent ingestion of test or control substances. The three dose groups consisted of: vehicle control (light paraffin oil) [Group I], diluted low-dose (50%) PEB Bottoms [Group II], high dose (100%) PEB Bottoms [Group III]. The appropriate doses or test control substance were applied topically to the prepared back of 5 test animals per group for a period of 6 hours. Treatment was performed once daily for a total of 5 doses.

Animals were observed daily for clinical signs, mortality and moribundity. Dermal reactions were observed and scored twice on the initial dosing day and at the time of residual test substance removal. The Draize Scoring System for evaluating dermal reactions was used for scoring purposes. Body weights were recorded immediately prior to initial treatment and again at necropsy. All animals surviving to the scheduled study termination were sacrificed on Day 8 and gross necropsies on all animals were performed.

**Results/Conclusions**

All animals survived to the termination of the study. No mortality occurred as a result of the 5-day repeated dermal application of Polyethylbenzene Bottoms to male and female rats at dose levels of 1.0 g/kg (Group II) and 2.0 g/kg (Group III). Statistical analyses of group mean body weights revealed weight losses among males and females at both the 1.0 and 2.0 g/kg dose levels that were significant at the 99% confidence level.

A yellow brown discoloration of the test site was seen among all animals treated with the test substance. Dermal irritation was observed among animals in Groups II and III. Barely perceptible erythema was observed in the Group II (1.0 g/kg) animals. Erythema (ranging from very slight to well defined) and barely perceptible edema were seen among animals in Group III (2.0 g/kg).

Focal thickening of the skin at the point of application of the test substance was observed in Group III (2.0 g/kg).

**Data Quality**

Reliability (Klimisch):  
Remarks:

2a  
Reliable with restrictions; acceptable, well-documented study report which meets basic scientific principles

**Reference**

Gulf Life Sciences Center. 1985. Five –Day repeated dose dermal toxicity study in rats of Polyethylbenzene Bottoms. Project No. 84-2137

**Other**

Last changed:  
Remarks:

October 20, 2003  
None